Dugga B 2019

TBMT37 / TBMT19

Please, write your Dugga-ID on all pages and your answers in Swedish or English. You need 12/15 points to pass.
Good luck! /Elin & Gunnar

1 Model formulation

Consider the following model

$$[\dot{A}] = -k1[A] \qquad [A](0) = 1 \qquad \hat{y} = ky[A]$$
$$[\dot{B}] = -k2[B] + k1[A] \qquad [B](0) = 0$$

(a) List all model states! (1 point)

(b) List all model parameters! (1 point)

(c) What can be measured? Explain in words. (1 point)

2 Model simulation and cost function

Consider the following model

$$[\dot{A}] = -k1[A] \qquad [A](0) = 4 \qquad k1 = 3$$

(a) Calculate $[A](0.1)$ with one step of Euler forward. (1 point)

(b) What happens with $[A]$ as time evolves? (1 point)

(c) What are the inputs and outputs of a cost function? (1 point)

3 Model formulation

Consider the following reactions

$$A \rightarrow B \tag{1}$$
$$A \rightarrow C \tag{2}$$
$$A \rightarrow \varnothing \tag{3}$$
$$C \rightarrow \varnothing \tag{4}$$

(a) Write down the differential equations that corresponds to these reactions. Assume mass action kinetics for reaction 2-4 and assume that reaction 1 has a saturation with respect to the concentration of A. Introduce parameters and initial conditions with values of your choice. (2 points)

(b) Add a measurement equation. You can measure something that is proportional to the sum of the concentration of A and C. (1 point)

4 Statistical tests

(a) Formulate the null hypothesis underlying a whiteness test (1 point)

(b) What do you conclude when you reject the null hypothesis in a $\chi 2$-test? (1 point)

(c) What do you conclude when you cannot reject a likelihood ratio test? (1 point)

5 Predictions and experimental design

A core prediction from a model structure/hypothesis has been tested experimentally, what can we conclude if:

(a) The experimental data with uncertainty lies within the predicted interval? (1 point)

(b) The experimental data with uncertainty lies far from the predicted interval? (1 point)

(c) How would the conclusion from (b) be different if the prediction is not known to be a core prediction? (1 point)

Answers: Dugga B 2019

1

(a) $[A], [B]$

(b) $k1, k2, ky, [A](0), [B](0)$

(c) The measurement equation, $\hat{y} = ky[A]$ shows that we can measure something that is proportional to the concentrations of A.

2

(a) $[A](0.2) = [A](0) + [\dot{A}](0)\Delta t = 4 + (-3 * 4) * 0.1 = 2.8$

(b) The concentration of A approaches 0 after a long time.

(c) The input is a set of parameters and the output is the agreement between model simulations and data

3

(a)

$$
\begin{aligned}
[\dot{A}] &= -\frac{Vmax[A]}{(Km + [A])} - k1[A] - k3[A] && [A](0) = 1 \\
[\dot{B}] &= \frac{Vmax[A]}{(Km + [A])} && [B](0) = 2 \\
[\dot{C}] &= k1[A] - k2[C] && [C](0) = 0 \\
k1 &= 3, k2 = 1, k3 = 4, Km = 2, Vmax = 0.1
\end{aligned}
$$

(b) $\hat{y} = ky([A] + [C])$

4

(a) The residuals between model and data are not correlated

(b) You conclude that the residuals are large compare to the data uncertainty and you therefore reject the null hypothesis (and the corresponding model structure)

(c) No conclusion

5

(a) You do not reject the model structure/hypothesis, instead the data supports your model structure.

(b) You reject the model structure/hypothesis. You know that you need to refine the model structure to be able to have an agreement with the new data.

(c) You cannot conclude anything, since you only reject the model with a particular set of parameters, and not the model structure/hypothesis.